JÜLICH
FORSCHUNGSZENTRUM

Computational Science at the Jülich Supercomputing Centre

Paul Gibbon

C2S@EXA Meeting, INRIA, Paris, 8 November 2016

HELMHOLTZ ASSOCIATION

JÜLICH FORSCHUNGSZENTRUM

Mission:

- Energy
- Climate
- Transport
- Health
- Key Technologies

FZ-Juelich:

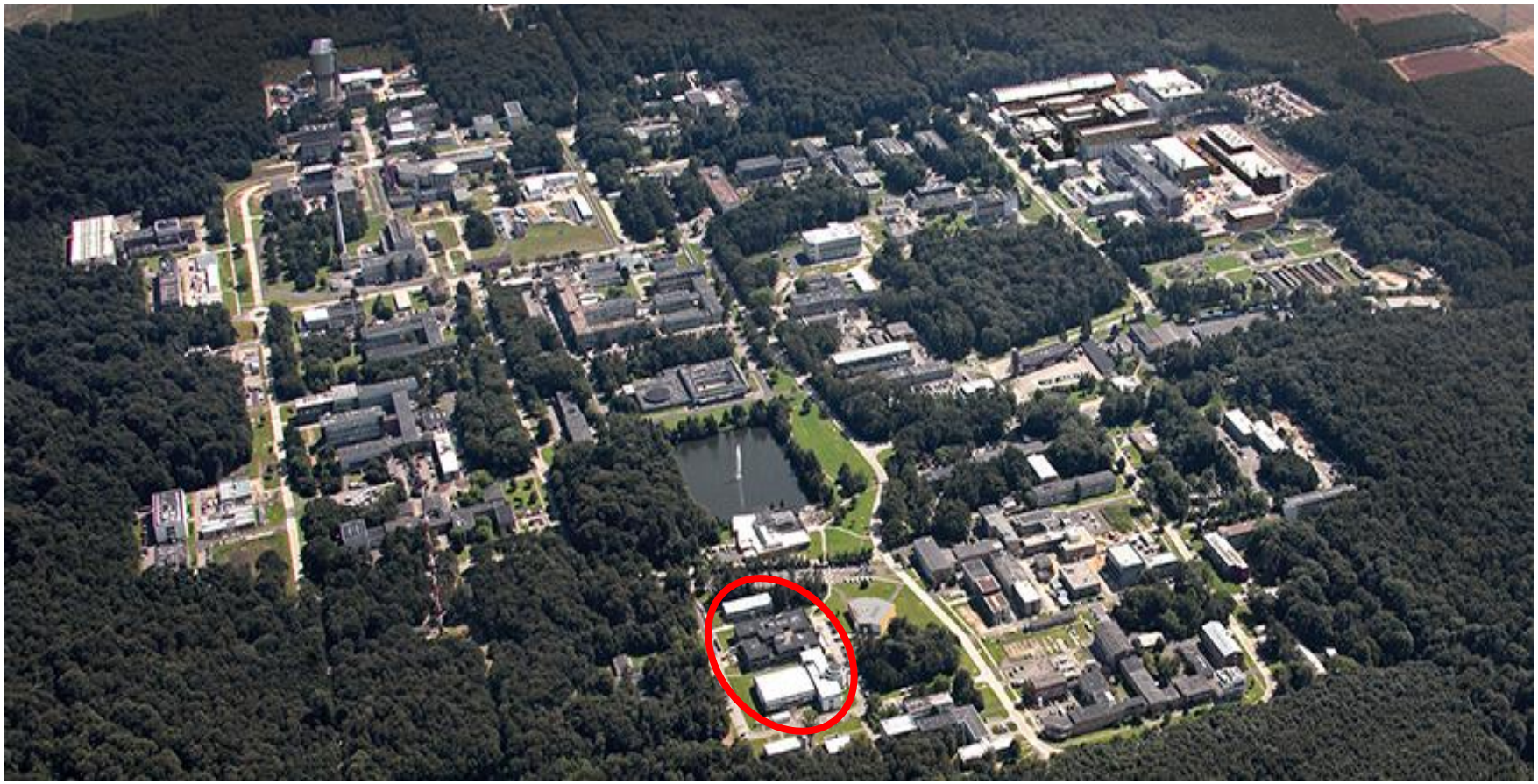
5800 staff

2000 scientists

800 PhD students

Budget: 600M€

Jülich Supercomputing Centre



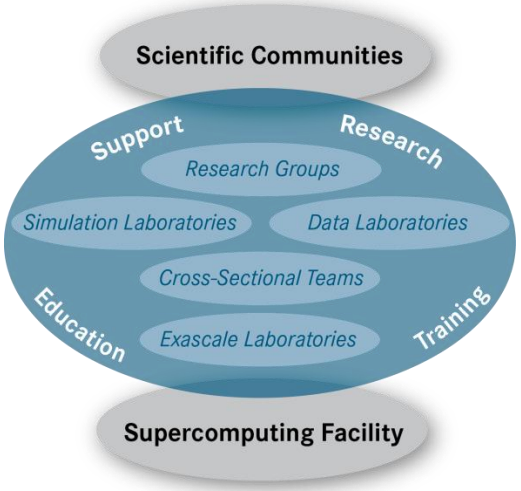
Jülich Supercomputing Centre

Supercomputer operation for:

- Centre – FZJ
- Region – RWTH Aachen University
- Germany – Gauss Centre for Supercomputing
  John von Neumann Institute for Computing
- Europe – PRACE, EU projects

Application support

- Unique support & research environment at JSC
- Peer review support and coordination



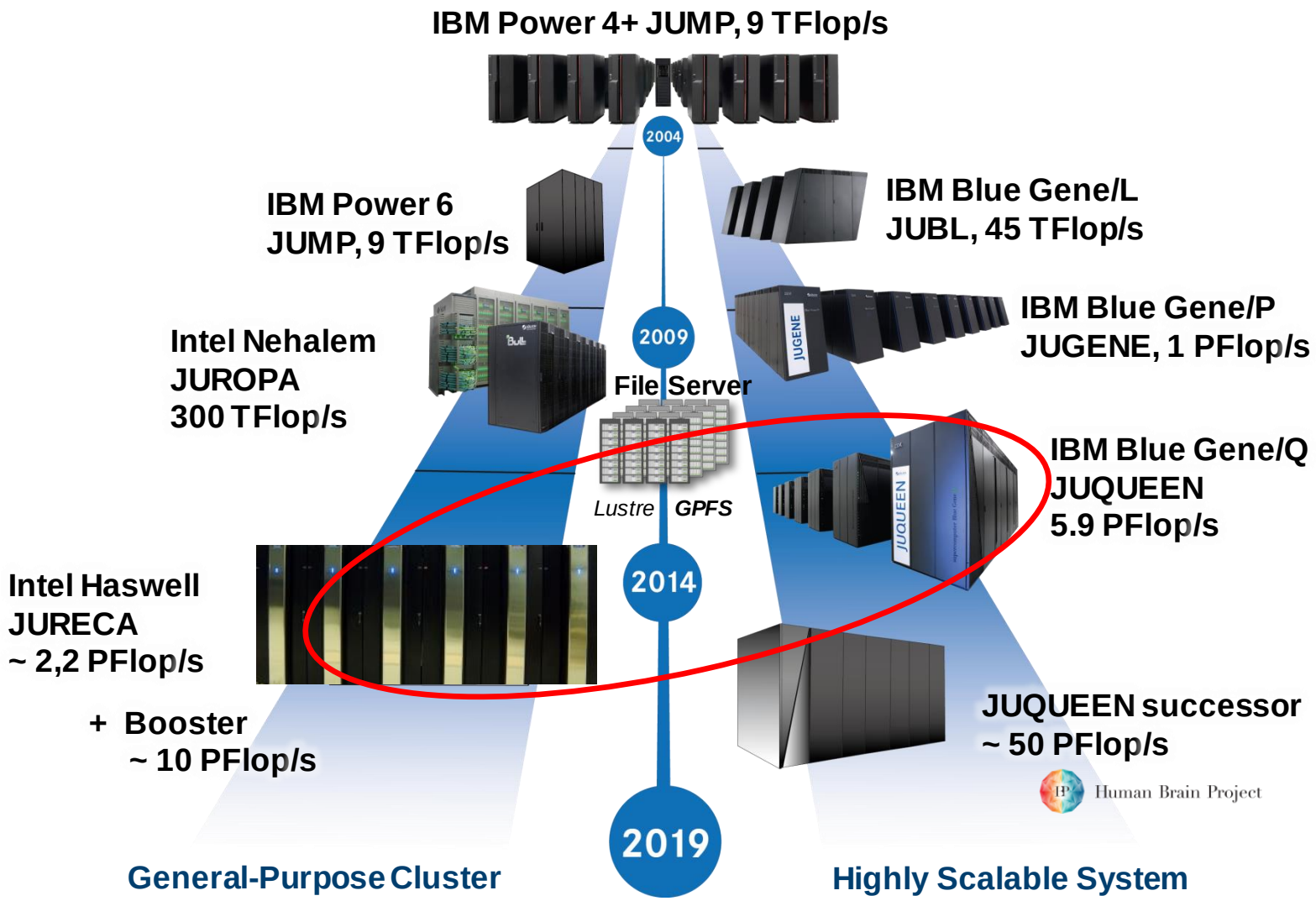
R&D work

- Methods and algorithms, computational science, performance analysis and tools
- Scientific Big Data Analytics with HPC
- Computer architectures, Co-Design
  Exascale Labs together with IBM, Intel, NVIDIA

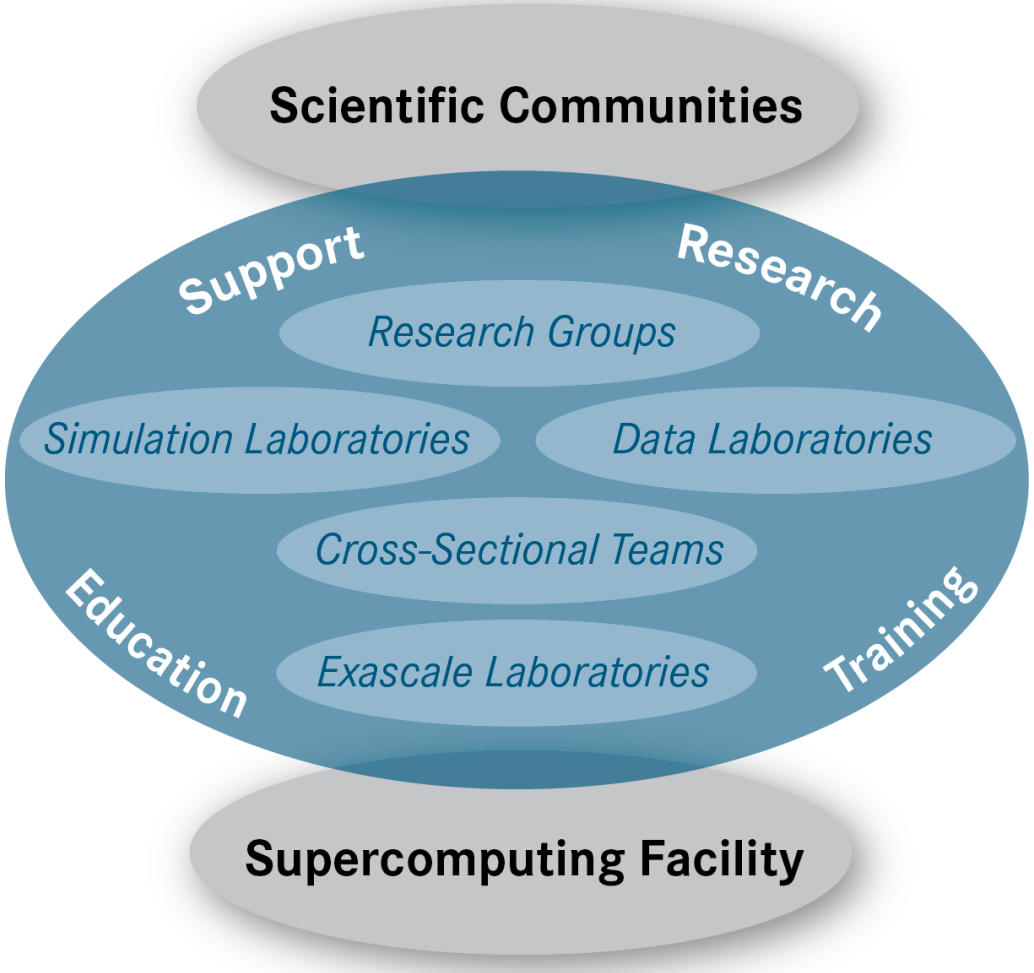
DEEP

Education and training

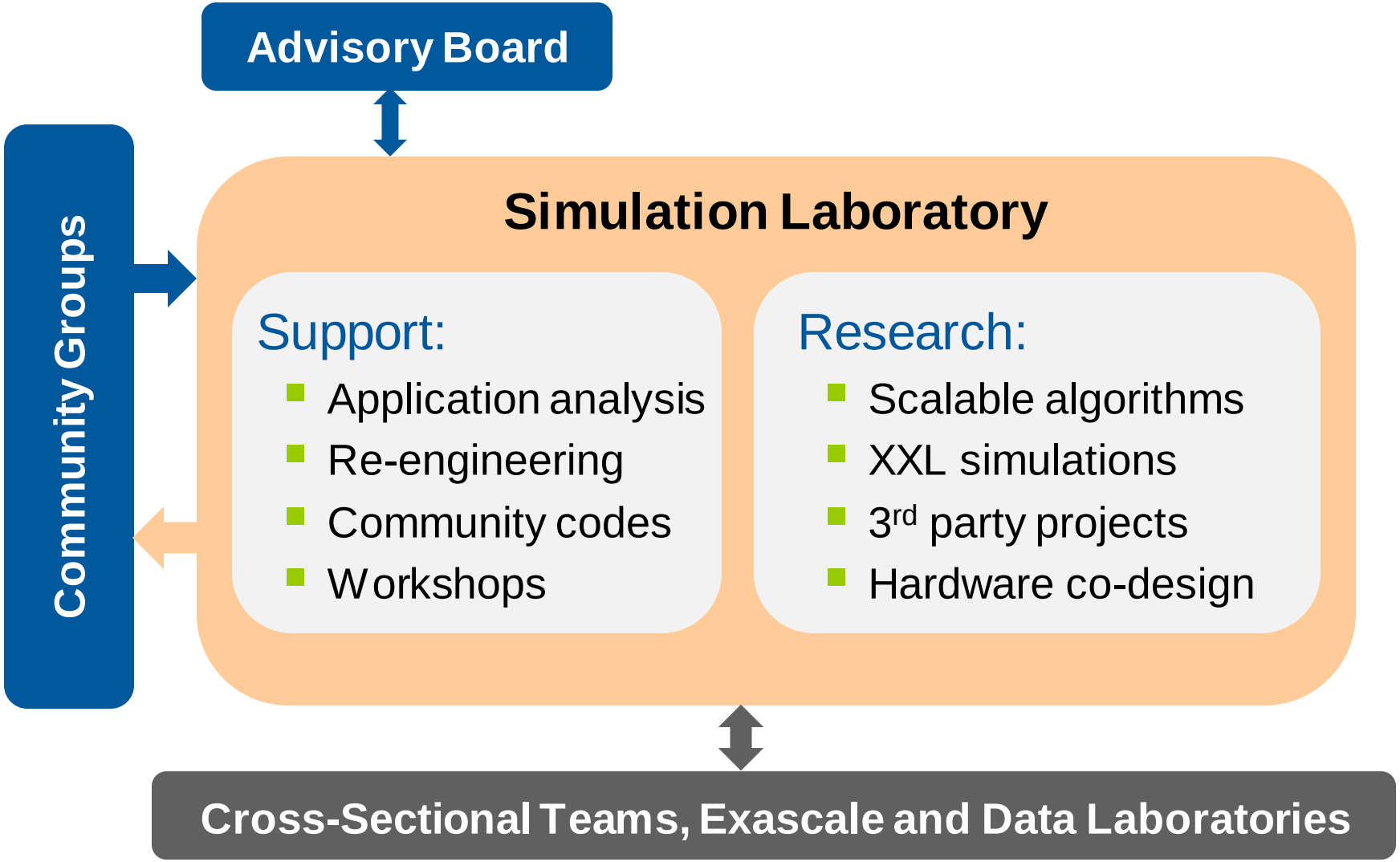
JSC Dual Architecture Strategy



Research and Support Environment



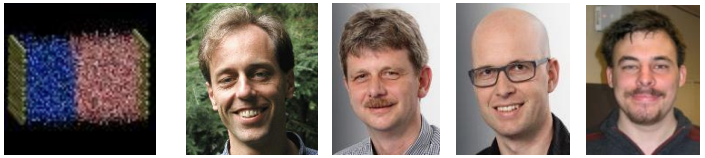
The Simulation Laboratory as HPC Enabler



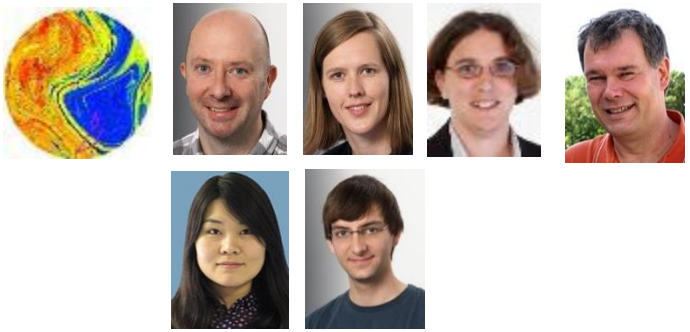
Simulation Labs @ JSC

Biology

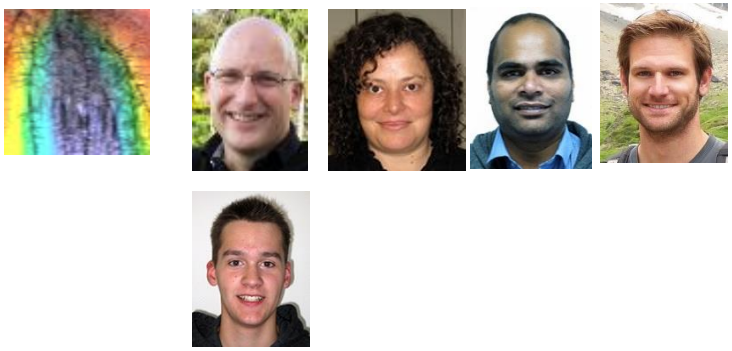
Molecular Systems



Climate Science



Terrestrial Systems



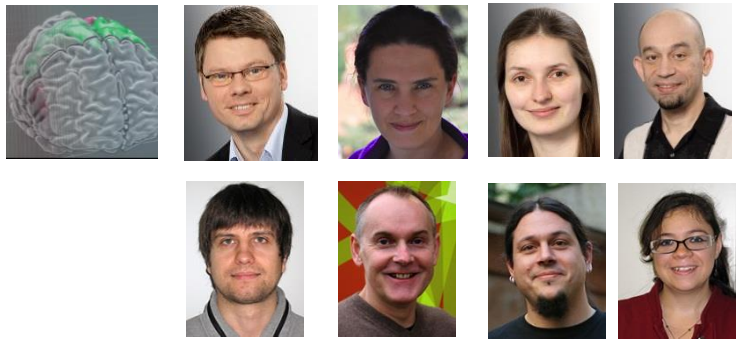
Nuclear & Particle

Fluid & Solid Eng.

Plasma Physics

Ab Initio Methods

Neuro-science



Applications

- Atomistic methods in materials science
- Computational biology
- Mesh-free plasma modelling
- Hydrology in terrestrial systems
- Linear solvers in Ab Initio computation
- Quantum information processing
- (Parallel in Time methods)

HPC in Materials Science

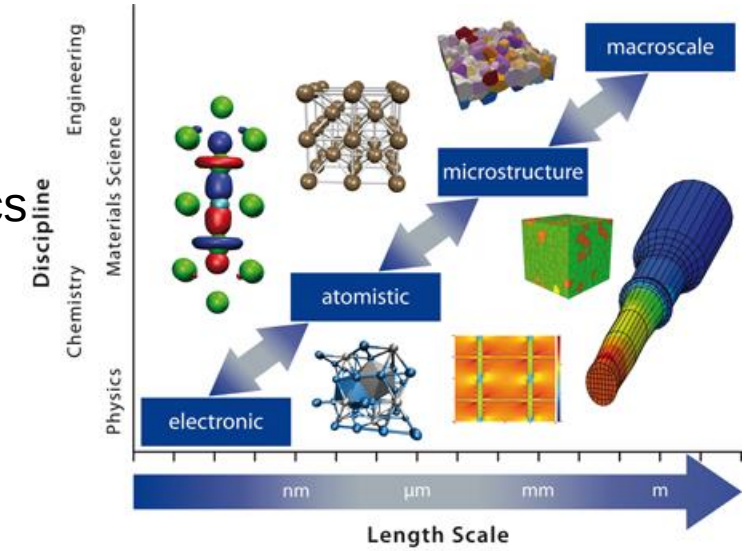
- Godehard Sutmann

- High Performance Computing on various length and time scales to extend range of applications in numerical experiments

JUQUEEN (Jülich)

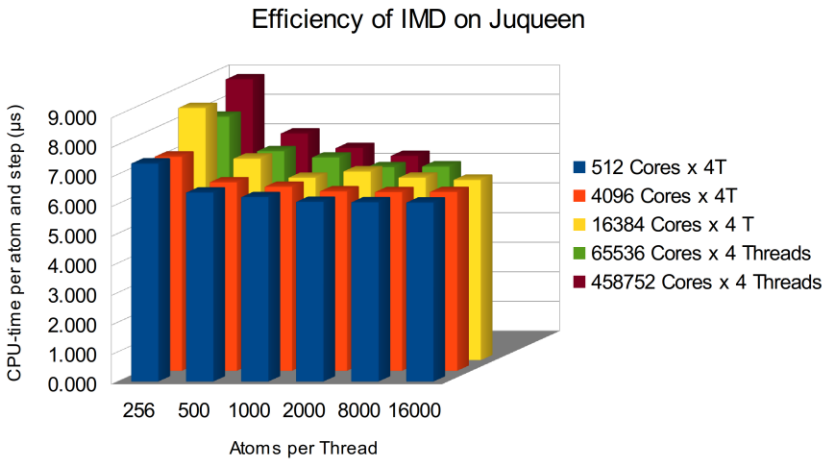

Vulcan (ICAMS)

- Atomistic methods
  - bond order potentials
  - embedded atom MD
  - force field based molecular dynamics
  - hybrid MD/Monte Carlo
- Mesoscopic methods
  - phase field
- Development of HPC methods



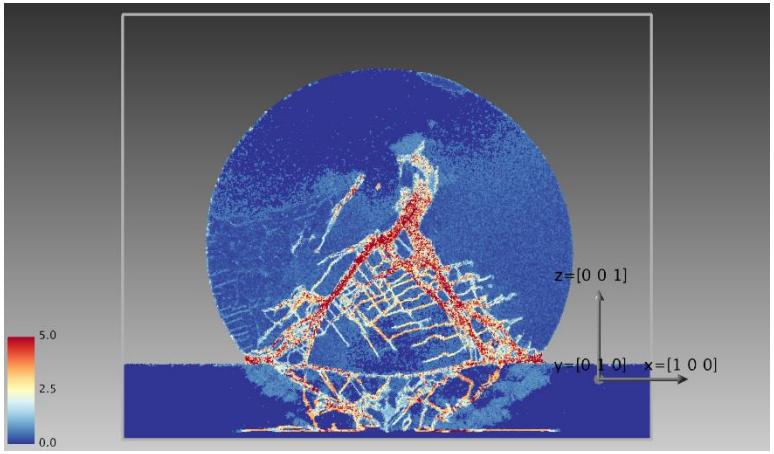
Molecular Dynamics IMD

- Very high efficiency obtained for **IMD** on JUQUEEN



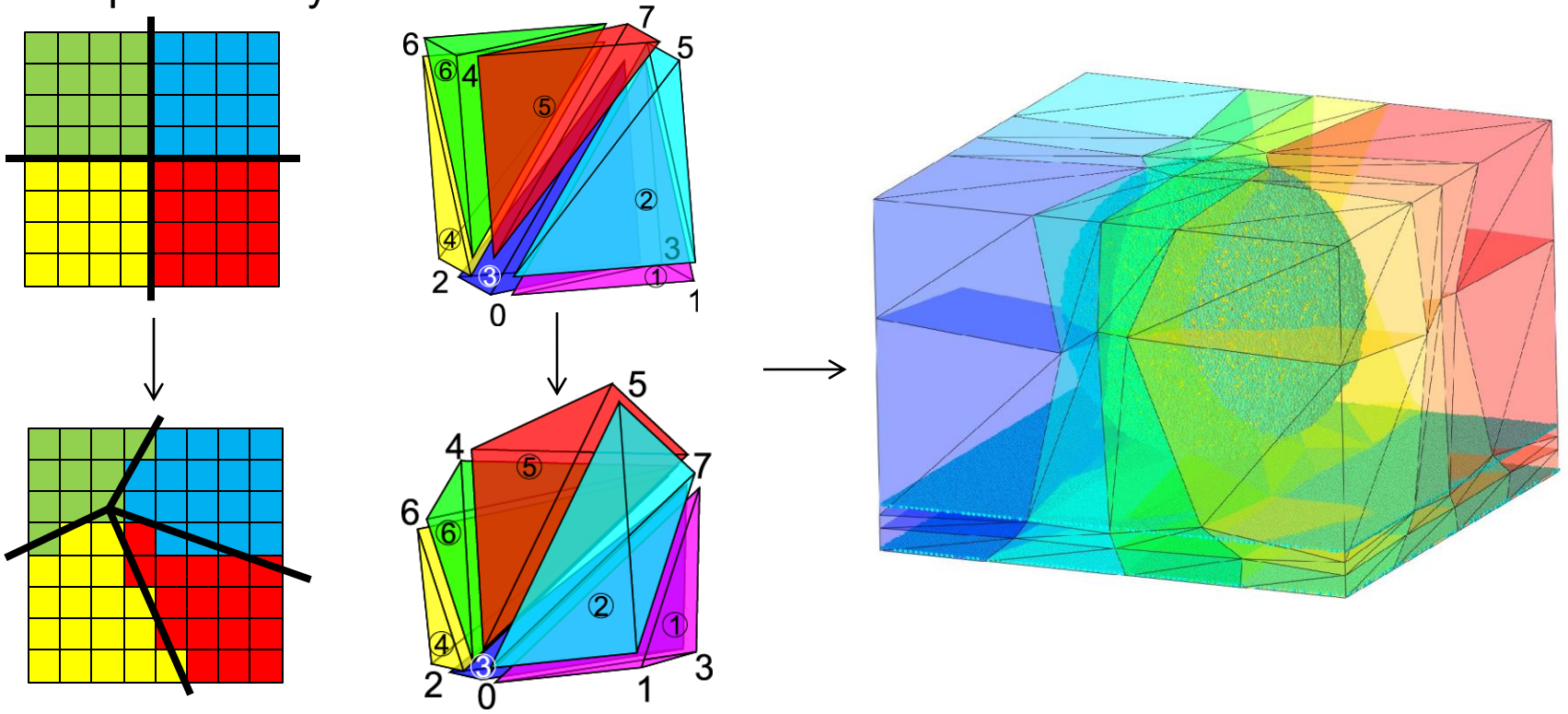
Scaling up to
458,752 JUQUEEN cores
using **1.835 Mio. Threads** (!)

- Enables simulations on large atomistic scales
  - Size effects in dislocation networks
  - Sub-micrometer particle deposition on surfaces



Adaptive load-balancing

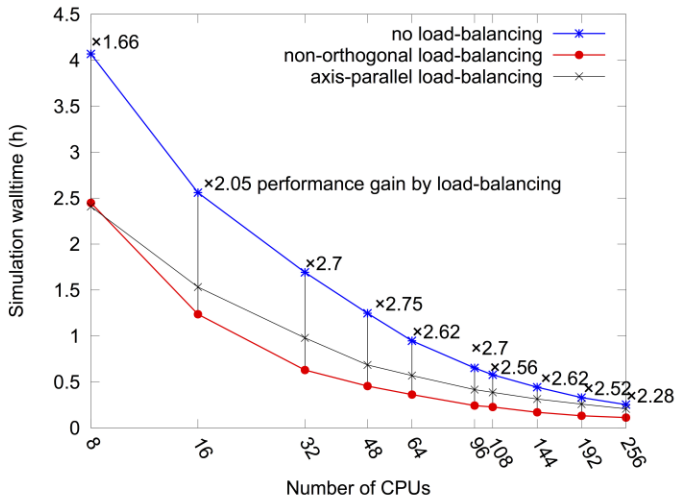
- Cell based deformation of computational domains – particles follow their container cells
- Adaptive LB by “force”-based motion of vertices

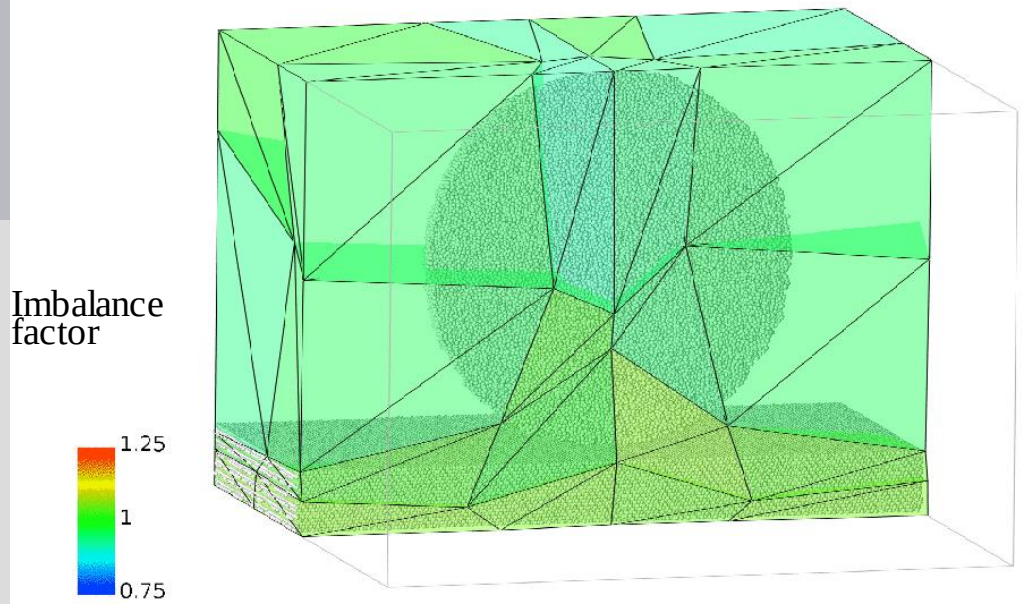


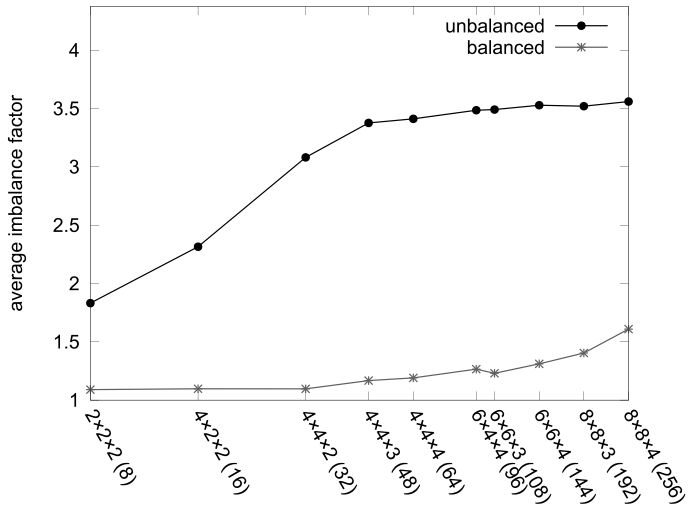
- Basic data and communication structures unchanged
- Disadvantage: Larger surface → possible communication overhead

Results

- Droplet simulation with ~1.000.000 atoms
  - 4x4x4 domains dynamically balanced
  - No extensive idle time on CPUs
- Integrated into OpenSource MD code IMD
- Method applicable to a wide range of particle simulation methods





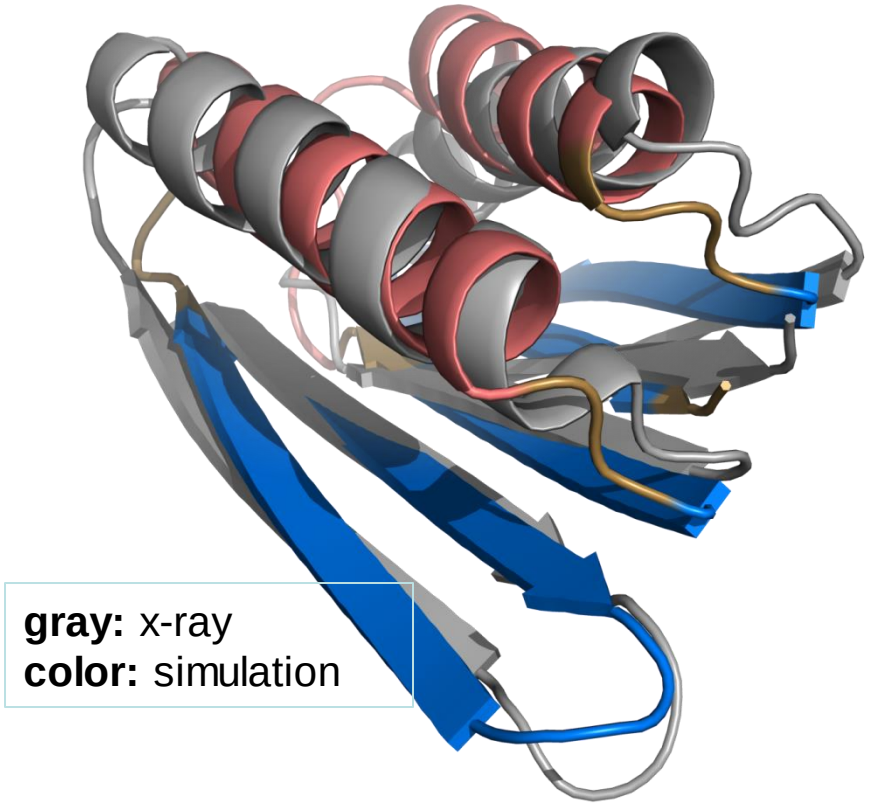


Computational Biology

– Olav Zimmermann

Top7: 92 amino acids, designed

- All-atom Replica Exchange Markov Chain Monte Carlo simulation using ProFASi
- ~ 20k CPU/h per folding event on JUROPA (cur. ~ 30 foldings)
- Free energy minimum at 3.5 Å from the experimental structure
- Largest protein folded ab initio
- Experimental folding time: ~ 1 s !!

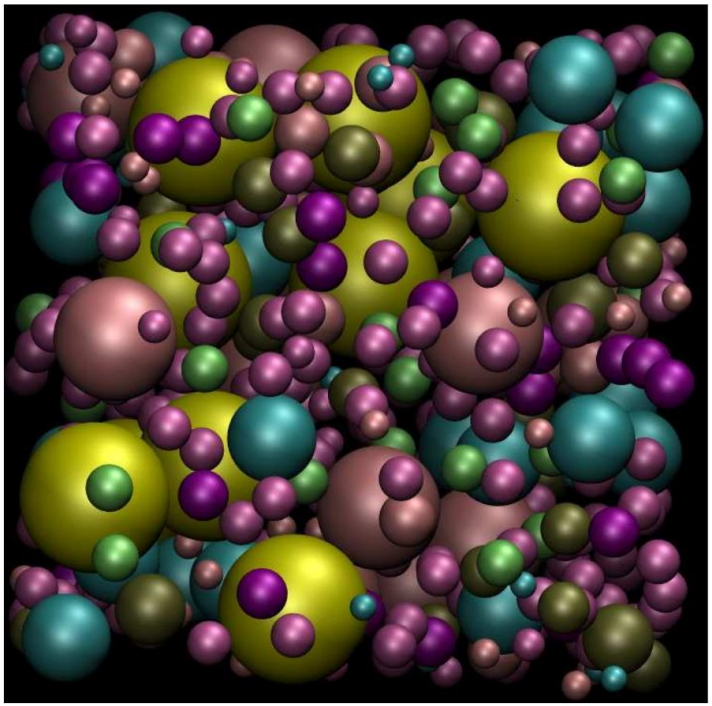


potential use in Biotechnology

- **SynBio:** Top7 used as enzyme scaffold, high thermostability

Biotech application

- **Partner:** FZJ_IBG-1 (W. Wiechert)
  E. v. Lieres, S. Kondrat
- **Project:** Multiscale modeling of 3D- reaction diffusion systems by combining Brownian Dynamics and Finite Element approaches.
- **Support goal:** Scaling to large numbers of processors to allow for relevant system sizes.
- **Applications:** exploration of spatial influences on biochemical reactions: crowding, natural and artificial compartments, enzyme immobilization, enzyme tethering.



Phys. Biol. **12** (2015) 046003 doi:10.1088/1478-3975/

Physical Biology

PAPER

The effect of composition on diffusion of macromolecules in a crowded environment

Svyatoslav Kondrat[1,3], **Olav Zimmermann**[2,3], **Wolfgang Wiechert**[1,3] **and Eric von Lieres**[1,3]

[1] Forschungszentrum Jülich, IBG-1: Biotechnology, 52425 Jülich, Germany
[2] Forschungszentrum Jülich, Jülich Supercomputing Centre, 52425 Jülich, Germany
[3] JARA — High-Performance Computing, Germany

E-mail: s.kondrat@fz-juelich.de

Least-Squared Optimized Poles (LSOP) eigensolver - Edoardo Di Napoli

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$A x = \lambda x$

Parallel linear solver: level 3

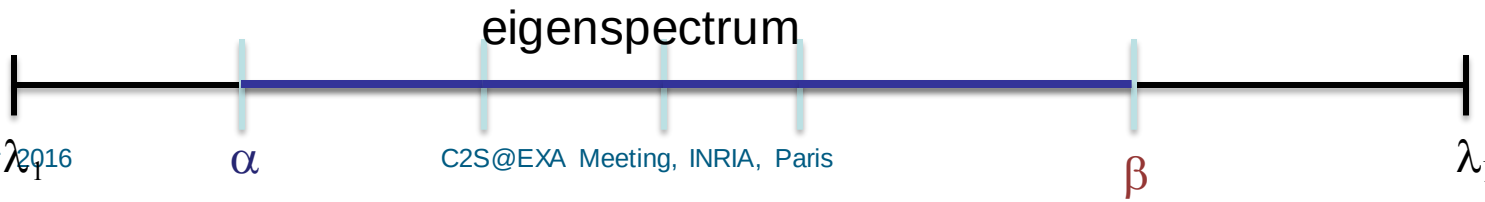
$$(A - Iz_i)\, V = Y$$

Parallelism over poles: level 2

$$\Sigma_i \alpha_i (A - Iz_i)^{-1}$$

Spectral projector: a rational function in complex plane

Parallelism over slices: level 1



Quantum Information Processing

- Kristel Michielsen

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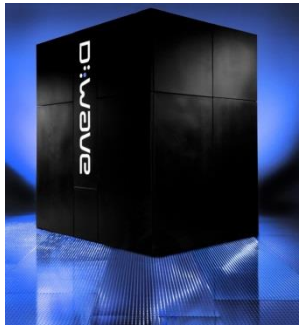
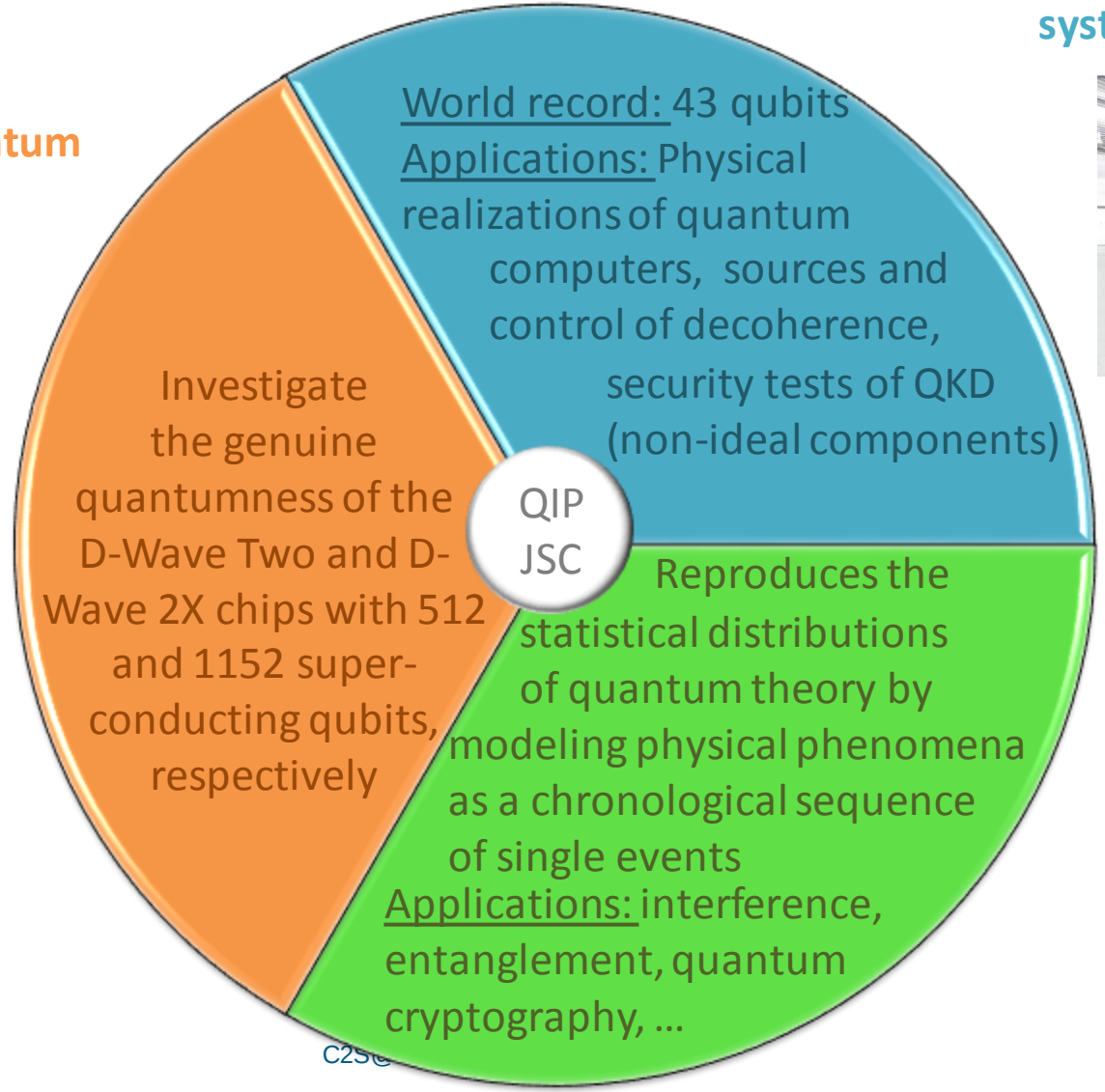
Large scale multi-qubit systems simulator

Adiabatic quantum computing



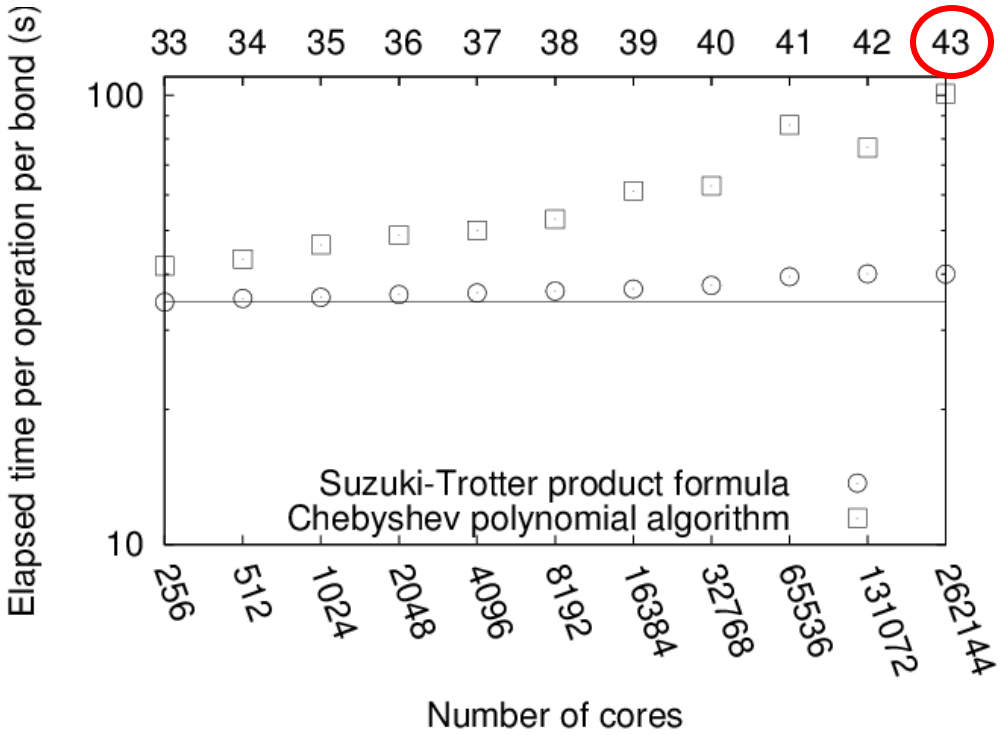


Discrete event simulation of QIP

Massively parallel quantum spin dynamics simulator

$$i\hbar \frac{\partial \Psi}{\partial t} = H\psi$$

N qubits → ψ is superposition of 2^N quantum states !



43 qubits: world record

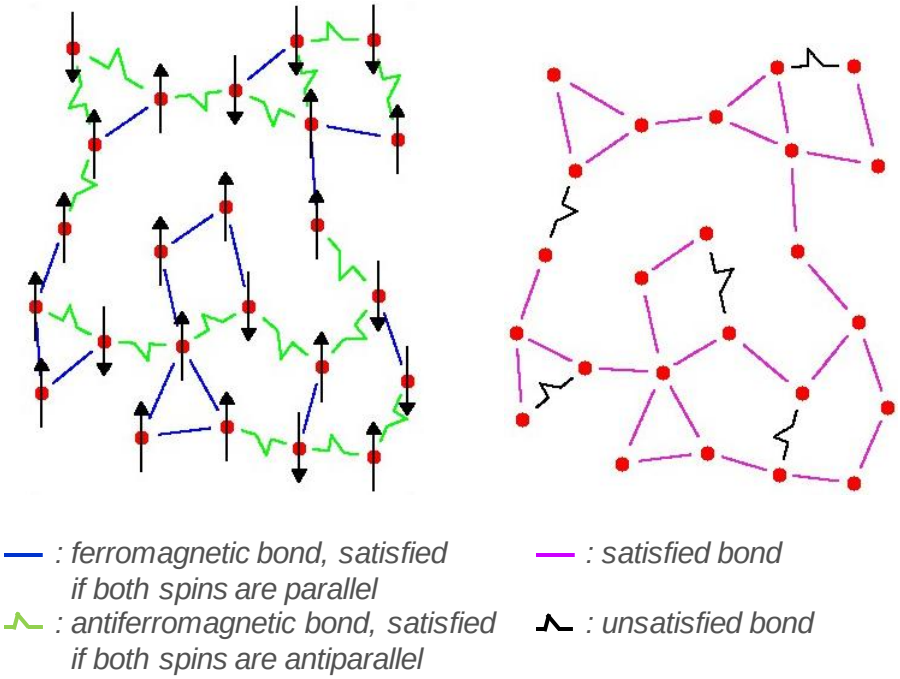
Comp. Phys. Comm. (2007),
Phys. Rev. B (2012), Phys. Rev. A (2013)

Applications: Physical realizations of quantum computers, sources and control of decoherence, security tests of quantum key distribution

Quantum annealing

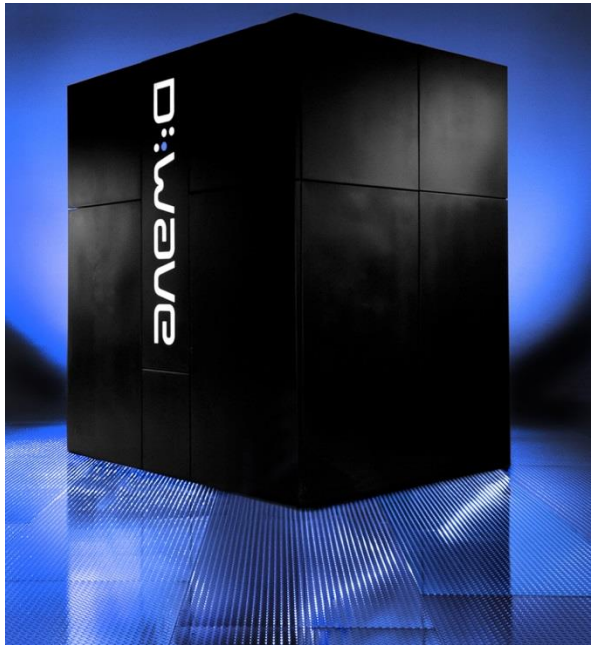
- Method using quantum fluctuations to search for the solution of an optimization problem.
- In physics, the search of the ground state of a spin-glass is a typical example of a hard optimization problem.

- Spin-glass: magnetic system with frustrated interactions

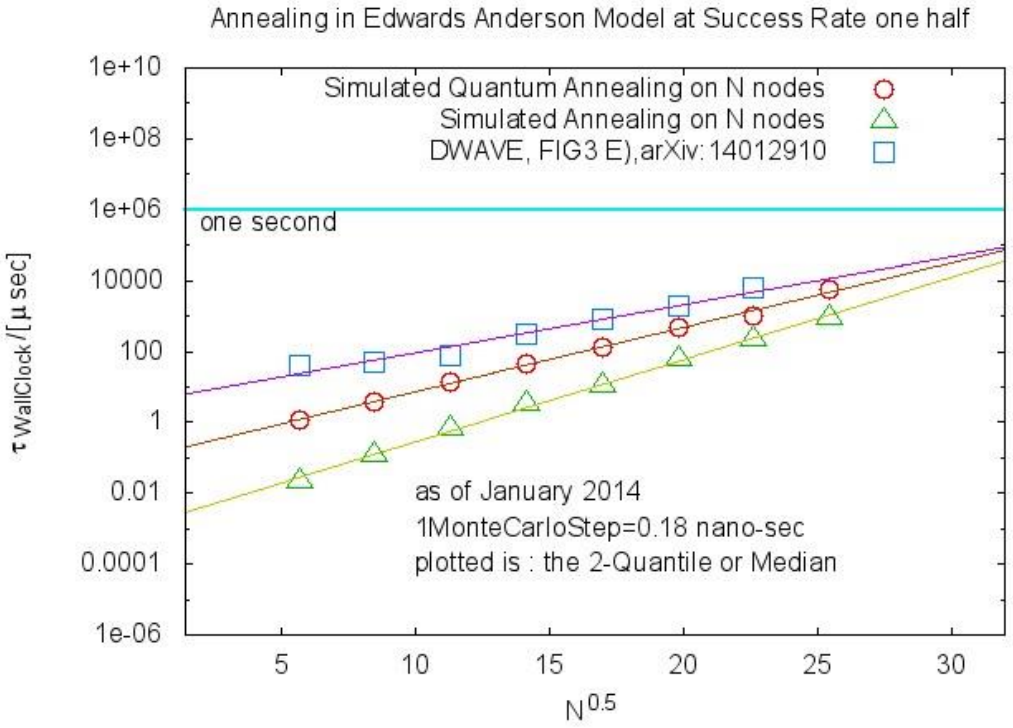


Quantum annealing

Benchmarking of a quantum annealing computer and (quantum) annealing simulators

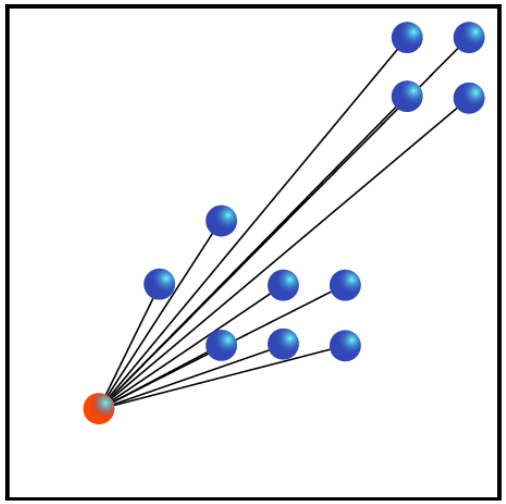


Quantum annealing computer manufactured by D-Wave



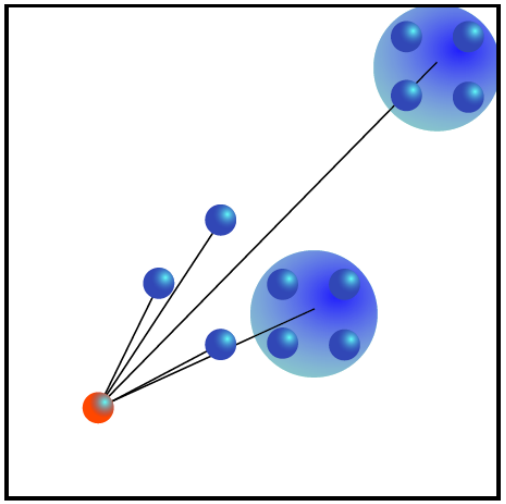
Mesh-free plasma simulation (P Gibbon): N-body problem with long-range potential

Direct Summation



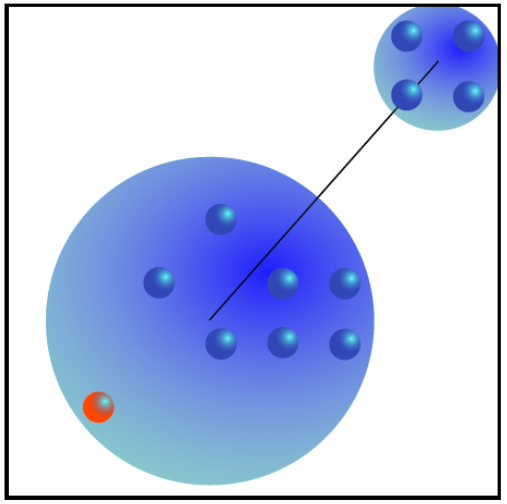
interactions: $\mathcal{O}(N^2)$

Treecode



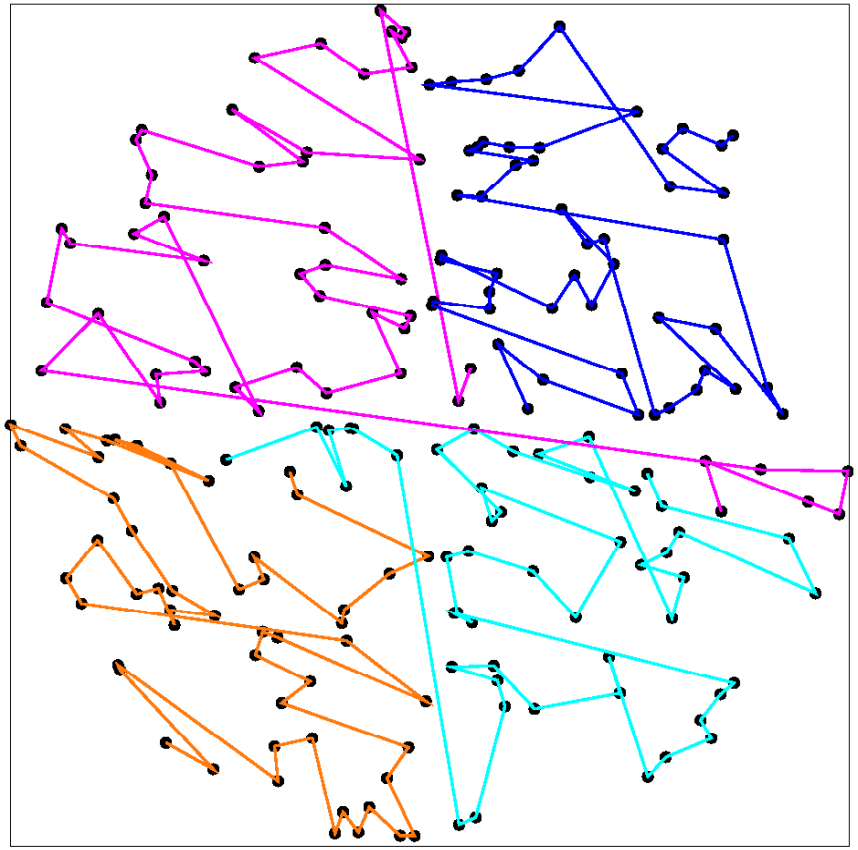
$\mathcal{O}(N \log N)$

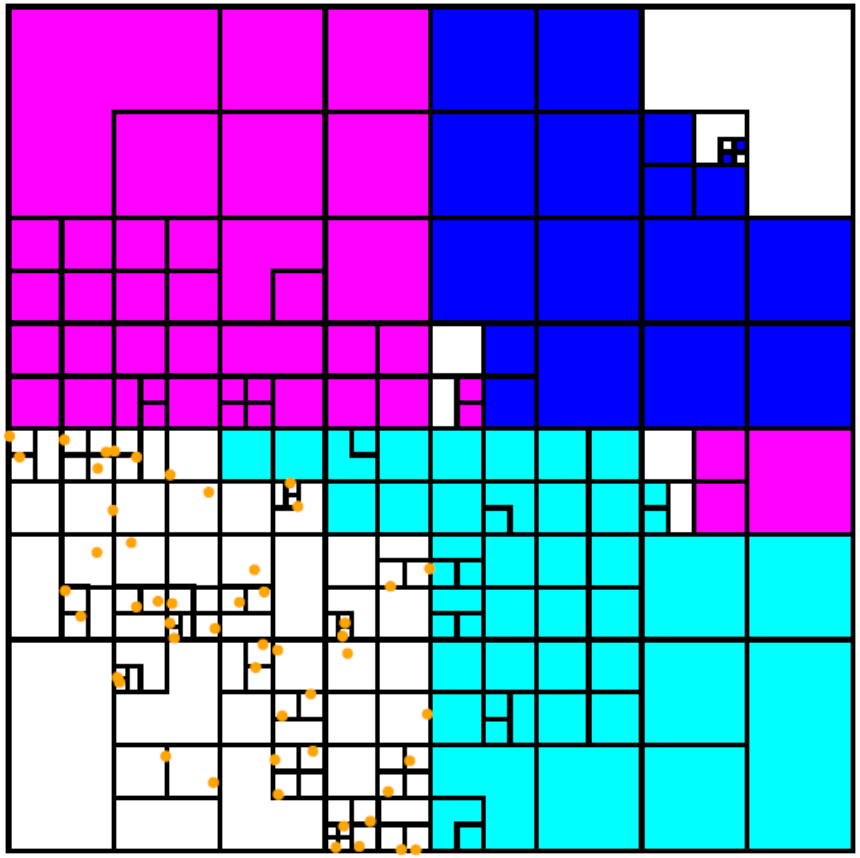
Fast Multipole Method



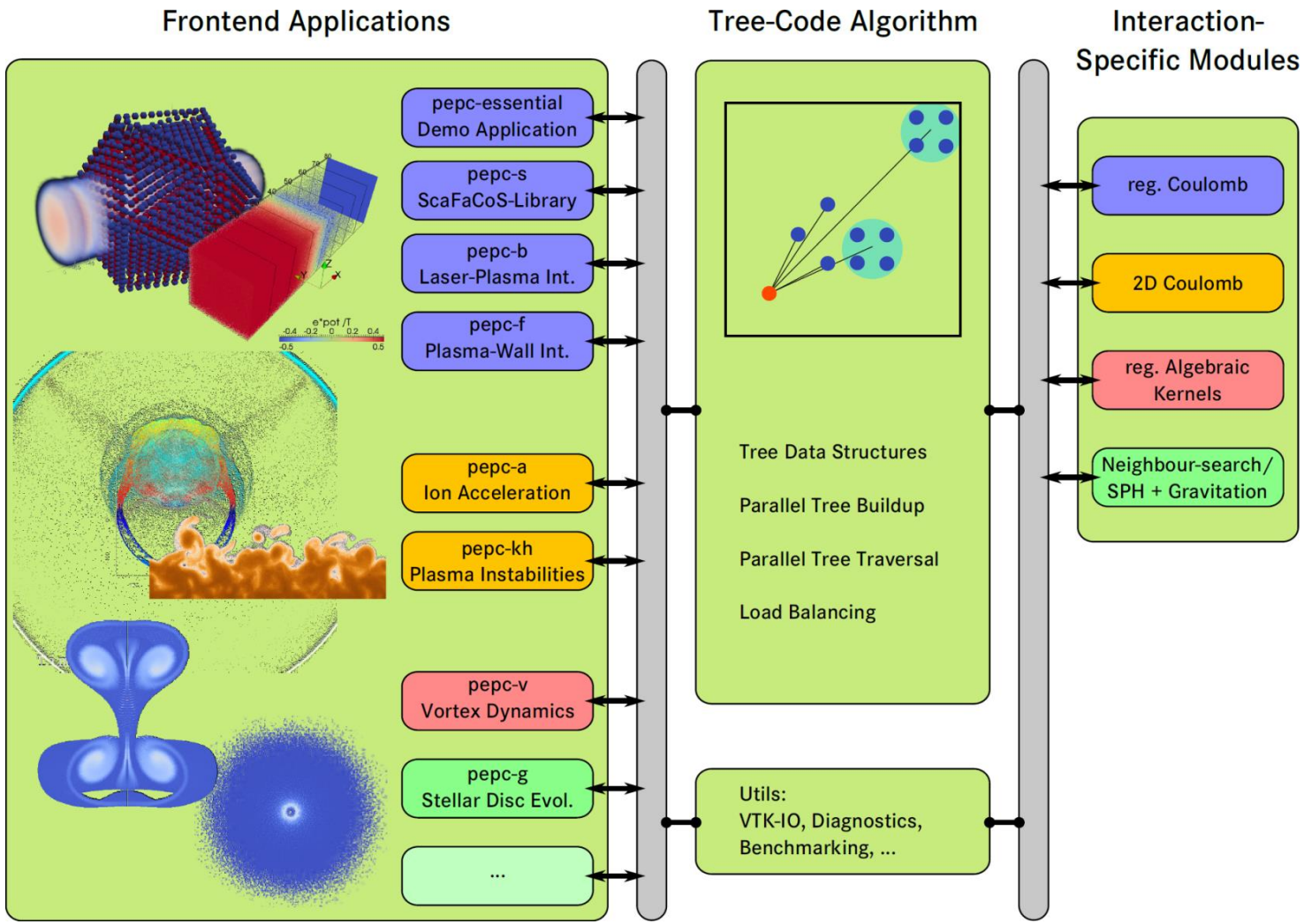
$\mathcal{O}(N)$

Parallel algorithm : space-filling curve

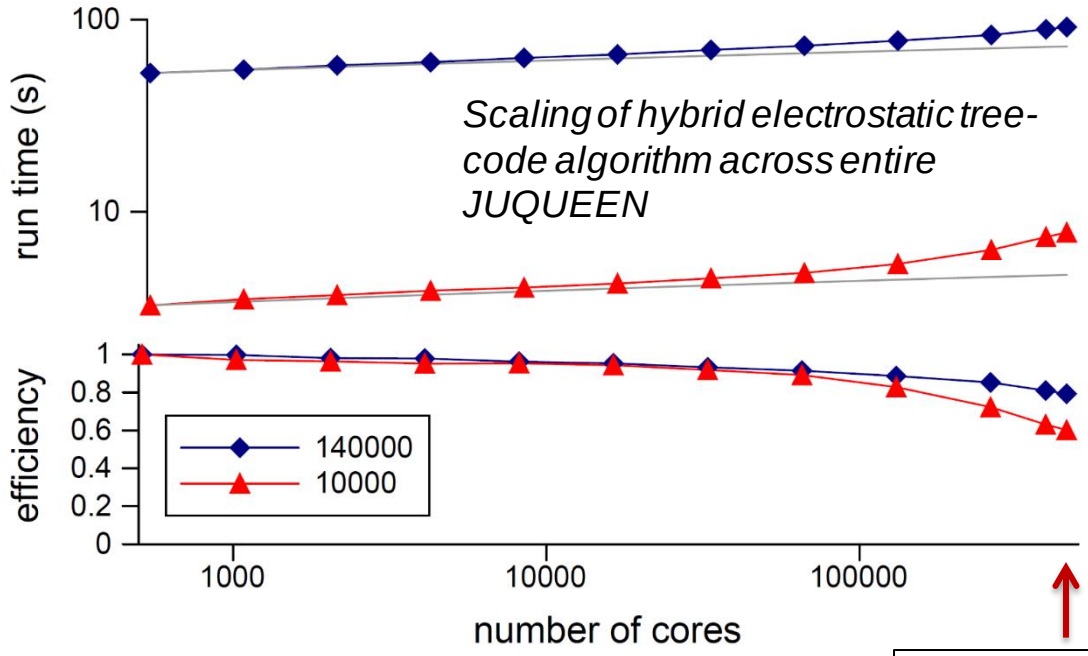


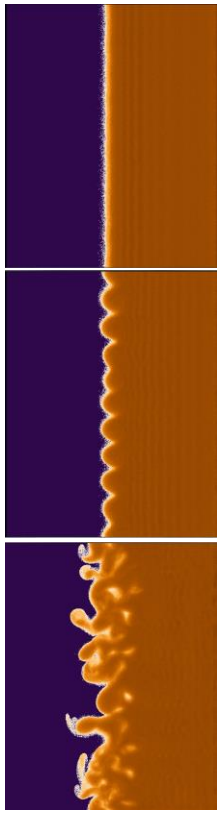


PEPC Framework: physics modules



Mesh-free plasma-wall particle simulation at scale





Kelvin-Helmholtz Instability in magnetised plasma

Steinbusch, B. ; Gibbon, P. ; Sydora, R. D. *Physics of plasmas* **23,** 052119 (2016)

Outlook: Mesh-free Darwin model

$$
\begin{aligned}
\nabla \cdot \mathbf{E}^{irr} &= 4\pi\rho \\
\nabla \times \mathbf{E}^{sol} &= -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{B} &= \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}^{irr}}{\partial t} + \cancel{\frac{1}{c}\frac{\partial \mathbf{E}^{sol}}{\partial t}}
\end{aligned}
$$

$$
\begin{cases}
\nabla^2 \varphi = -4\pi\rho \\
\nabla^2 \mathbf{A} = -\dfrac{4\pi}{c}\mathbf{J}^{sol}
\end{cases}
$$

Poisson-like field-solver

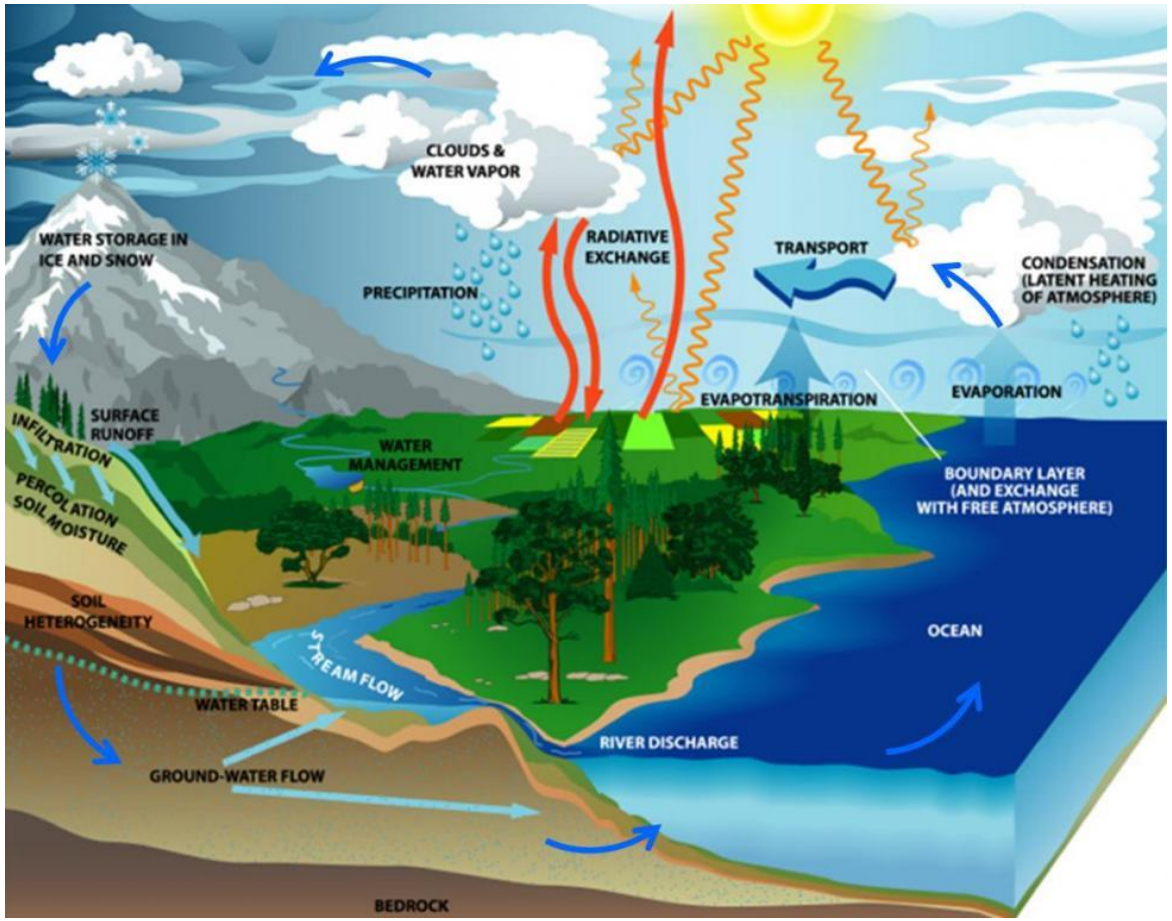
Implicit integrator

$$
\begin{cases}
\dot{\mathbf{P}}_i = -\dfrac{\partial \mathcal{H}_i}{\partial \mathbf{x}_i} = -q_i \nabla \varphi(\mathbf{x}_i, t) + \dfrac{q_i}{c}\nabla\big(A(\mathbf{x}_i, t)\cdot \mathbf{v}\big) \\
\dot{\mathbf{x}}_i = \dfrac{\partial \mathcal{H}_i}{\partial \mathbf{P}_i} = \dfrac{1}{m_i \gamma_i}\left[\mathbf{P}_i - \dfrac{q_i}{c}\mathbf{A}(\mathbf{x}_i, t)\right] = \mathbf{v}_i
\end{cases}
$$

L. Siddi, G. Lapenta, PG, *Physics of plasmas* (in prep., 2017)

Terrestrial systems:

- Klaus Görgen

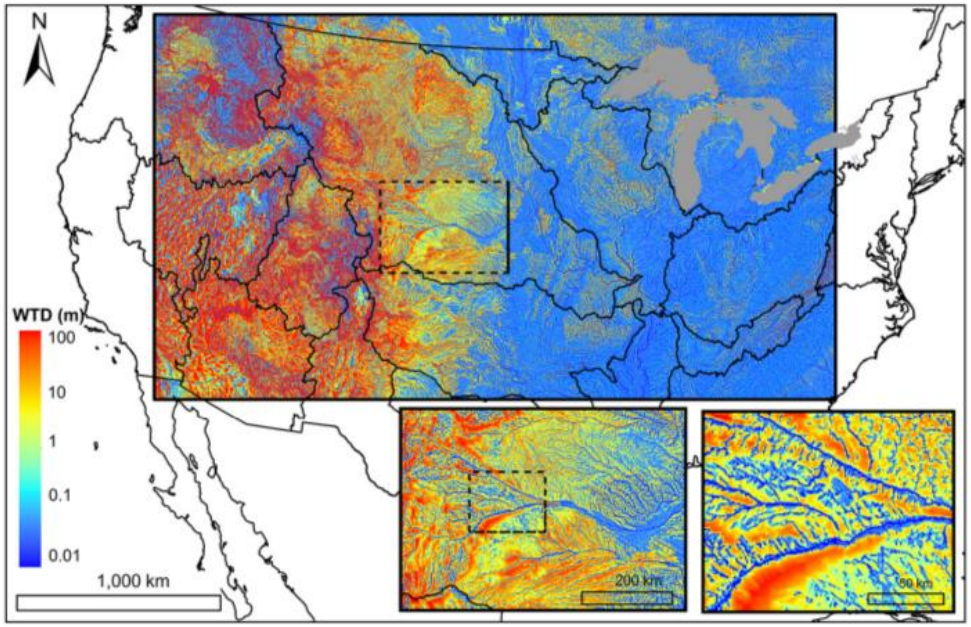


http://www.esrl.noaa.gov

Complex interactions and feedbacks between various sub-systems of the geo-ecosystem (e.g. pedo-, bio-, hydro- or atmosphere) at a multitude of spatio-temporal scales

Anthropogenic climate system changes modify land surface and ecosystem processes with impacts on may sectors (e.g. water management, argriculture, power generation)

ParFlow hydrologic model

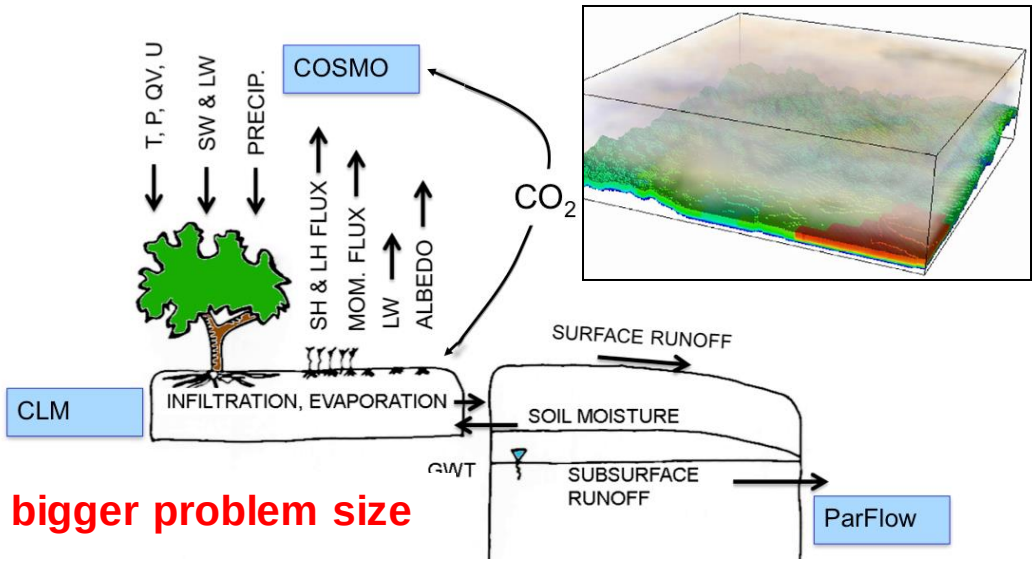


Map of water table depth (m) over continental USA with two insets zooming into the North and South Platte River basin, headwaters to the Mississippi River. Colors represent depth in log scale (from 0.01 to 100 m). Maxwell et al 2015

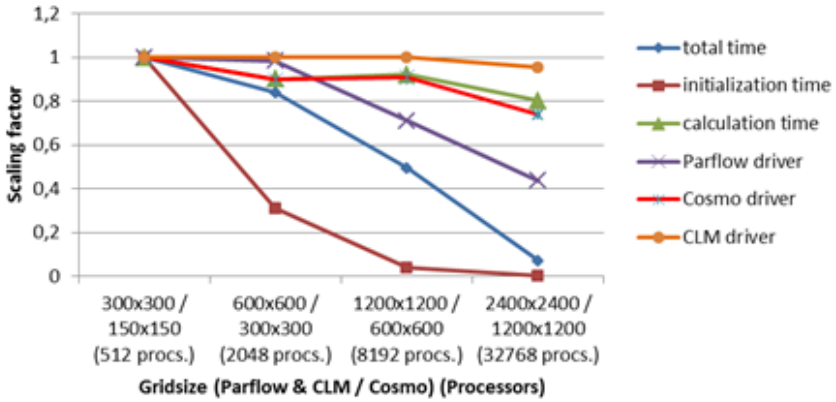
Simulates surface and subsurface flow: highly resolved simulations afford the identification of patterns across multiple space scales and new approaches in water resources assessment

Coupled model system TerrSysMP

- Fully integrated multi-physics simulation platform, towards earth system models at regional scale, multi-disciplinary research tool
- Current primary focus: water cycle
- Complex real-world patterns are resolved
- Conceptual "virtual realities" aid in process understanding

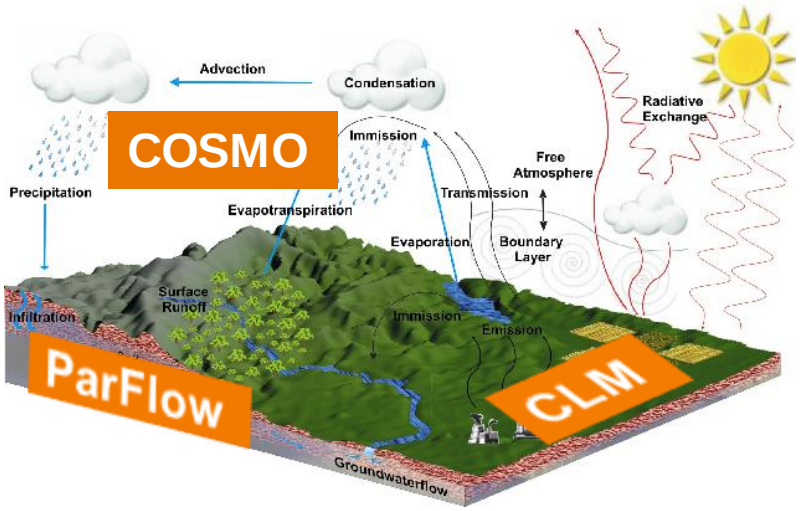


BG/Q scaling: 32768 procs => 64 x bigger problem size



- Use of highly flexible external coupler OASIS
- Refactoring of coupling interface towards extreme scaling
- Close coop with Parallel Performance team
- Collaboration with FZJ IBG-3, Uni Bonn (MIUB)
- Exploration of new HPC architectures

First Successes

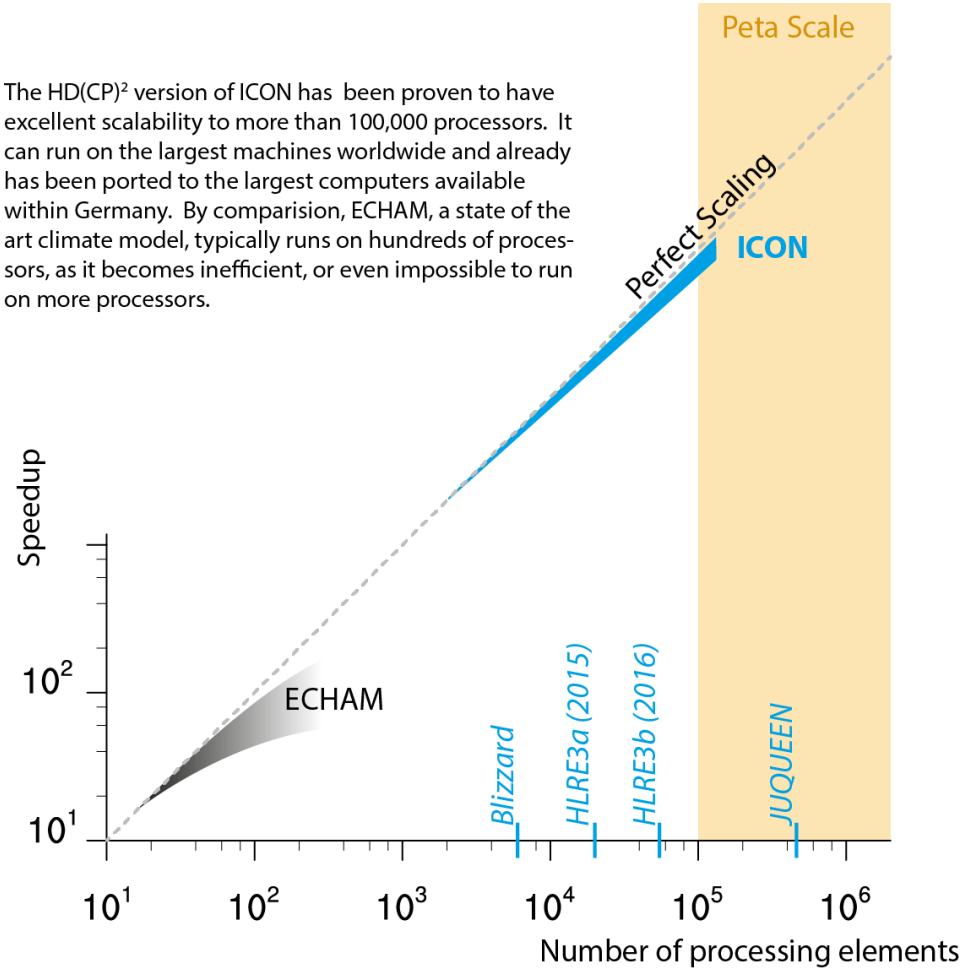


- Refactoring of OASIS-MCT coupling interface to remove scaling bottleneck
- Scaling now to 32k cores: 64x increased problem size!

HPSC TerrSys

A B C/J geoverbund aachen bonn köln jülich

The HD(CP)² version of ICON has been proven to have excellent scalability to more than 100,000 processors. It can run on the largest machines worldwide and already has been ported to the largest computers available within Germany. By comparision, ECHAM, a state of the art climate model, typically runs on hundreds of processors, as it becomes inefficient, or even impossible to run on more processors.



High-Q Club

- Dirk Brömmel

Start a collection of codes to showcase running on all 28 racks of Blue Gene/Q at JSC, effectively using all 458 752 cores with up to 1.8M hardware threads

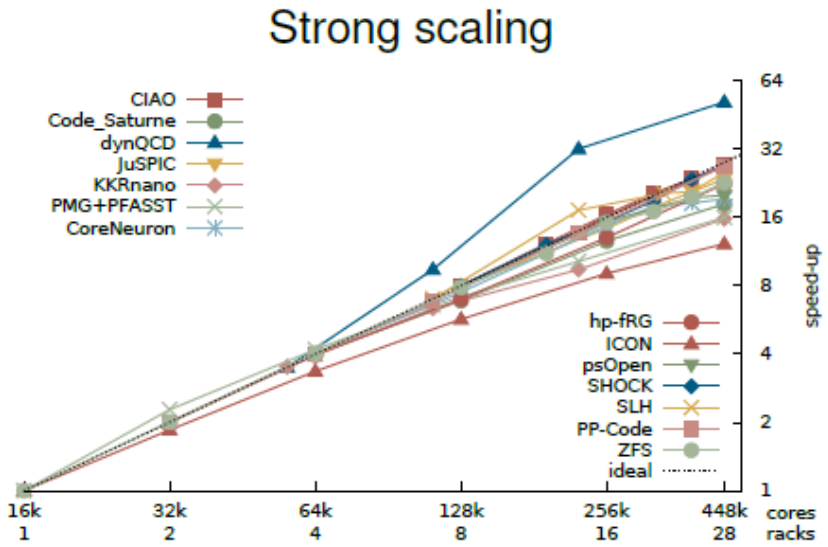
⟶ Promote the idea of exascale capability computing

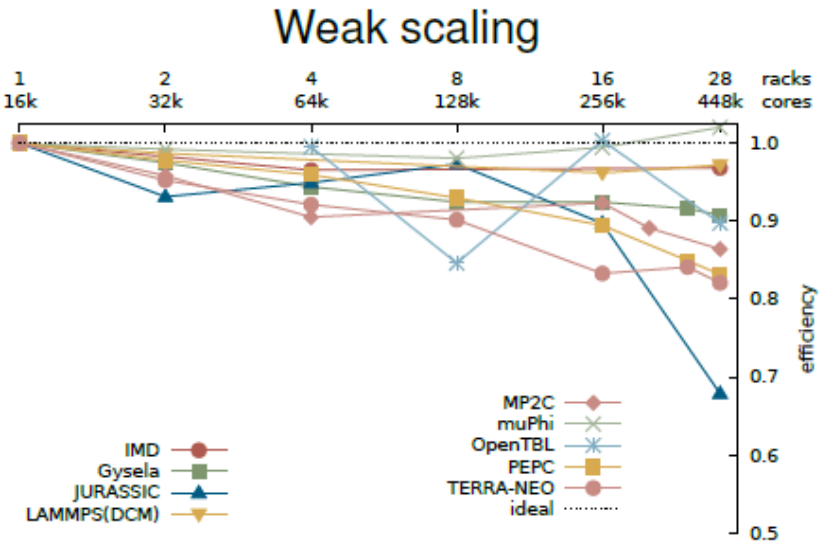
⟶ Spark interest in tuning and scaling codes

Goal

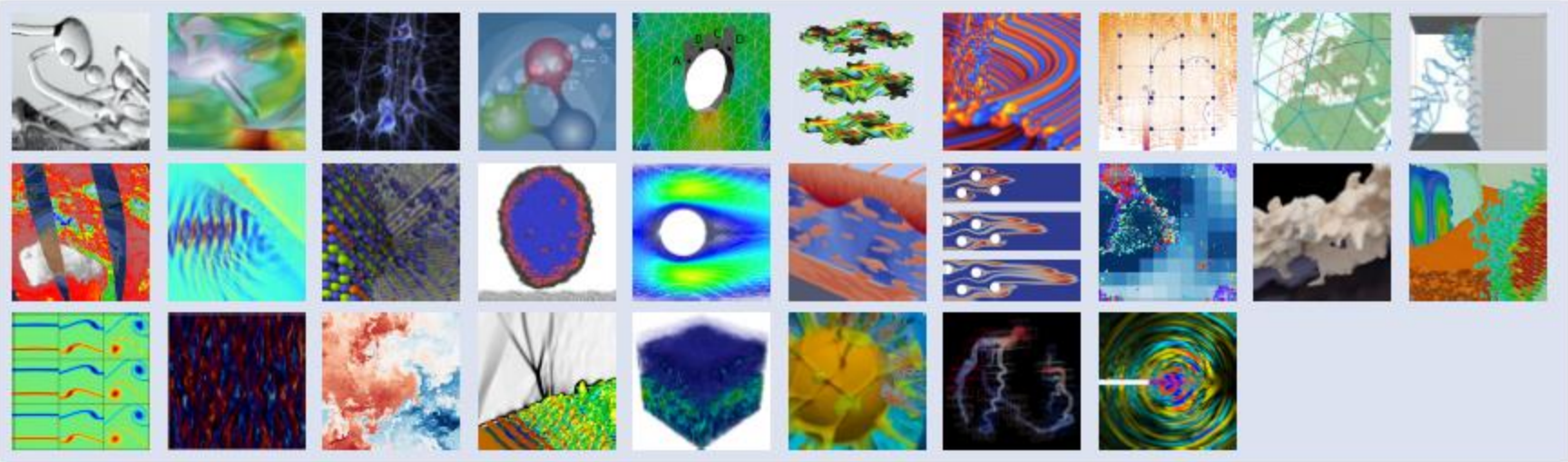
- Encourage our users to try and reach exascale readiness
- Establish milestones in application development towards future systems
- Identify and understand bottlenecks in trying to reach millions of threads/processes and learn how to transition to exascale systems

High-Q scaling results



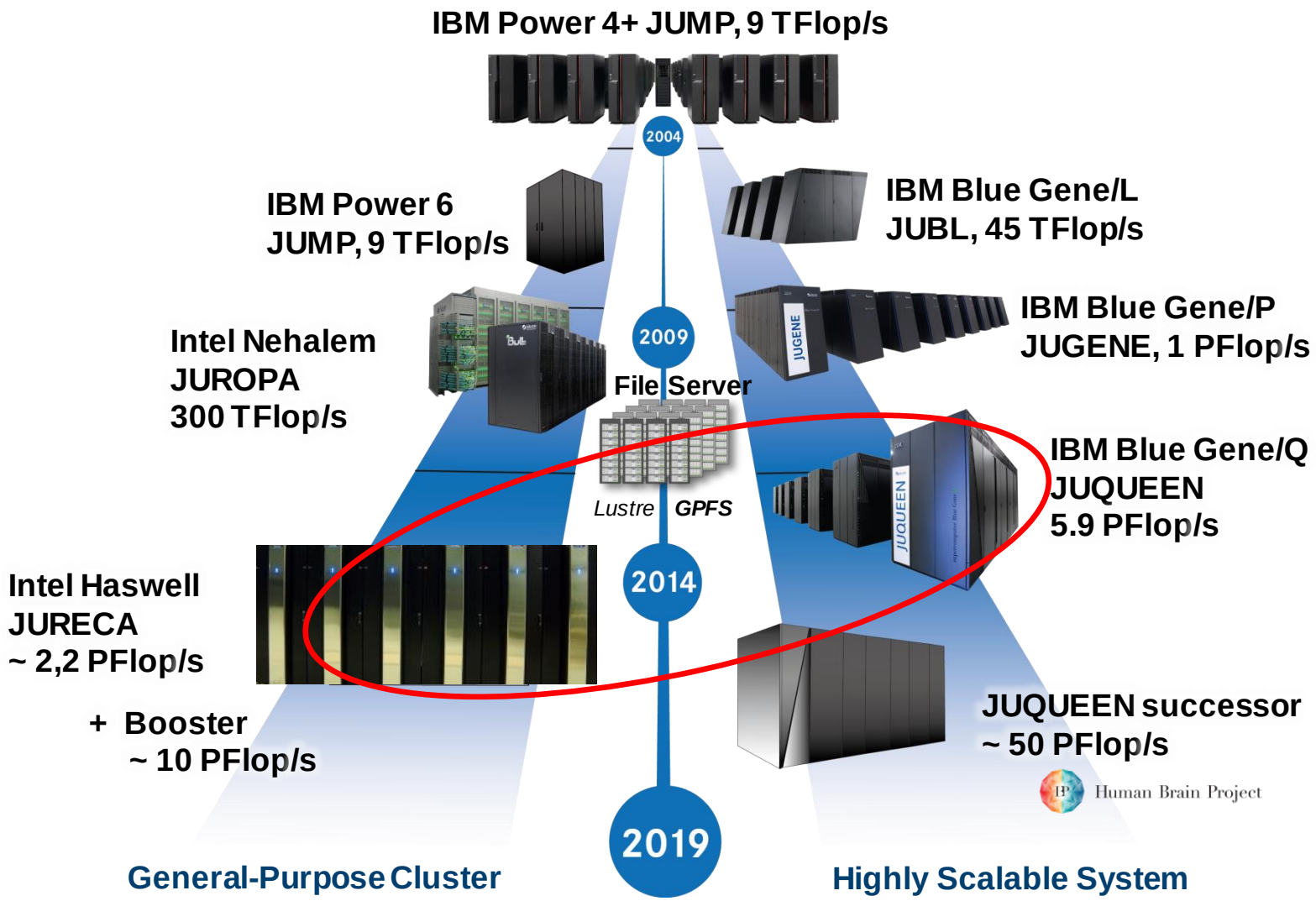


Current membership



CIAO, Code_Saturne, CoreNeuron, dynQCD, FE2TI, FEMPAR, Gysela, hp-fRG, ICON, IMD, JURASSIC, JuSPIC, KKRnano, LAMMPS(DCM), MP2C, $\mu\varphi$ (muPhi), Musubi, NEST, OpenTBL, PEPC, PMG+PFASST, PP-Code, psOpen, SHOCK, Seven-League Hydro, Terra-Neo, waLBerla, ZFS

JSC Dual Architecture Strategy



JSC's Architecture Strategy – Rationale

Dilemma #1

- Grand Challenge applications require extreme performance
- Not achievable with general purpose architectures (x86 Clusters): Cost, Energy
- Highly scalable architectures not suitable for applications requiring high single node performance, large memory per core

Solution: Dual architecture approach

- JUQUEEN - Highly scalable system
- JUROPA / JURECA – general purpose system
- Common Storage

JSC's Architecture Strategy – Rationale

JÜLICH FORSCHUNGSZENTRUM

Dilemma #1

- Grand Challenge applications require extreme performance
- Not achievable with general purpose architectures (x86 Clusters): Cost, Energy
- Highly scalable architectures not suitable for applications requiring high single node performance, large memory per core

Solution: Dual architecture approach

- JUQUEEN - Highly scalable system
- JUROPA / JURECA – general purpose system

Dilemma #2

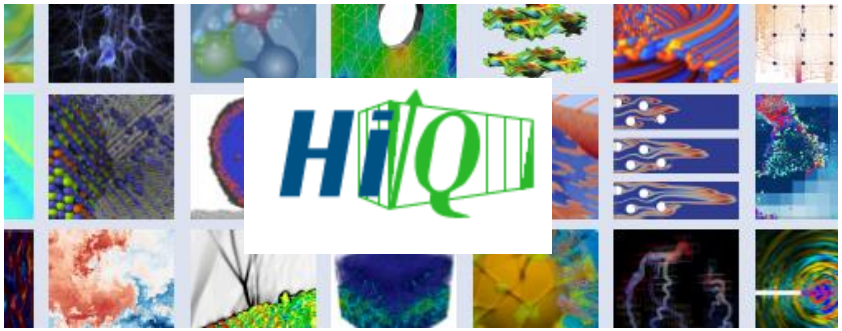
- Parts of complex applications often have different requirements and scalability properties
- Heterogeneous architectures / clusters with accelerators: static ratio of CPU / Accelerator performance potentially wastes resources and energy

Solution: Cluster – Booster concept

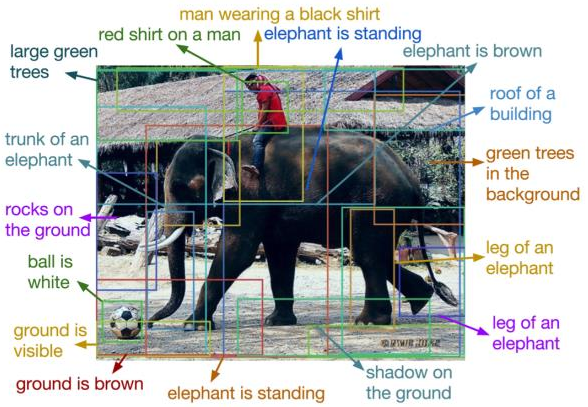
- Separation of CPU (Cluster) and Accelerator (Booster) allows dynamic resource allocation to optimize resource utilization
- Requires substantial application modifications

More Diverse Challenges …

Extreme Scale Computing



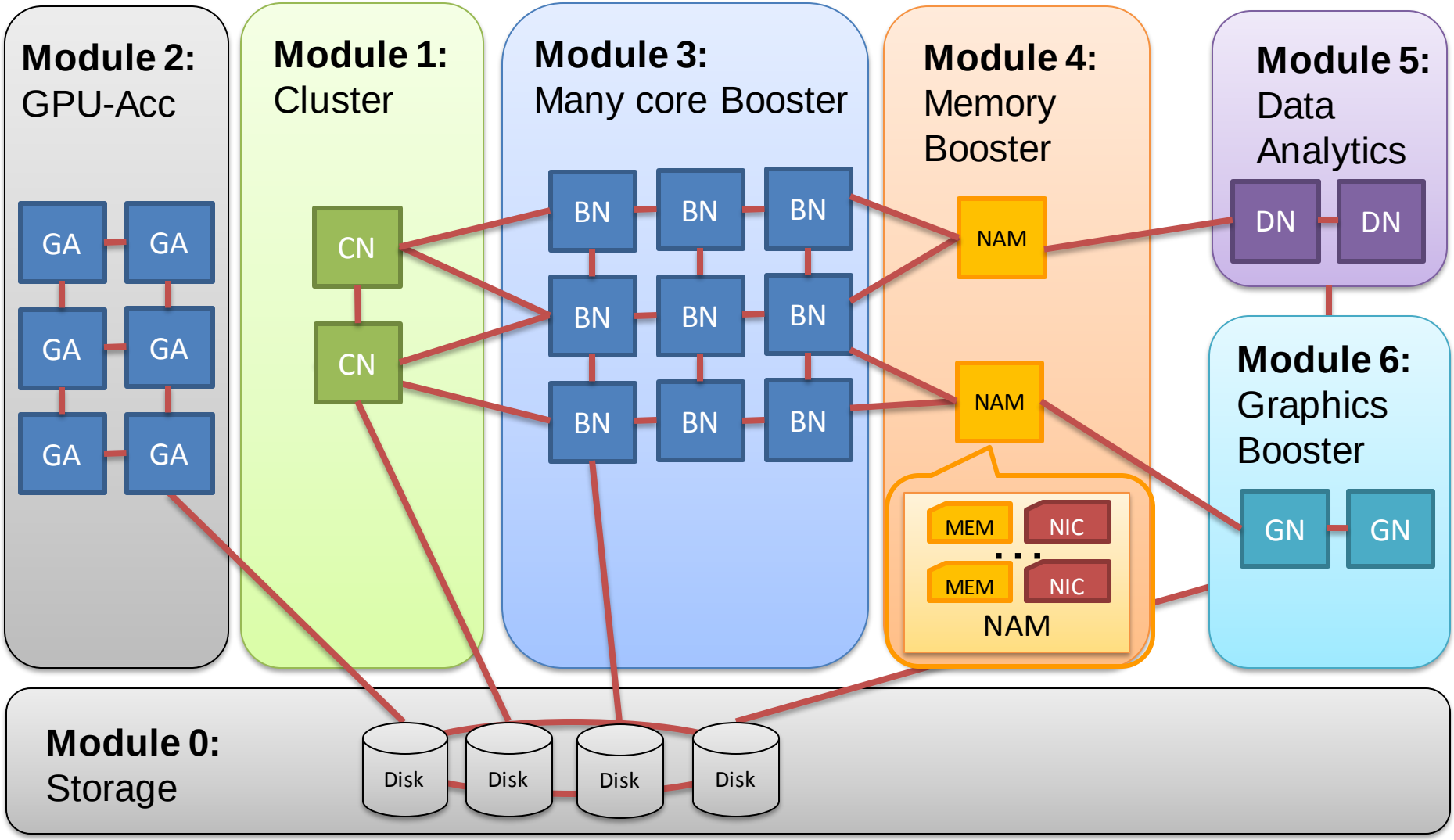
Deep Learning



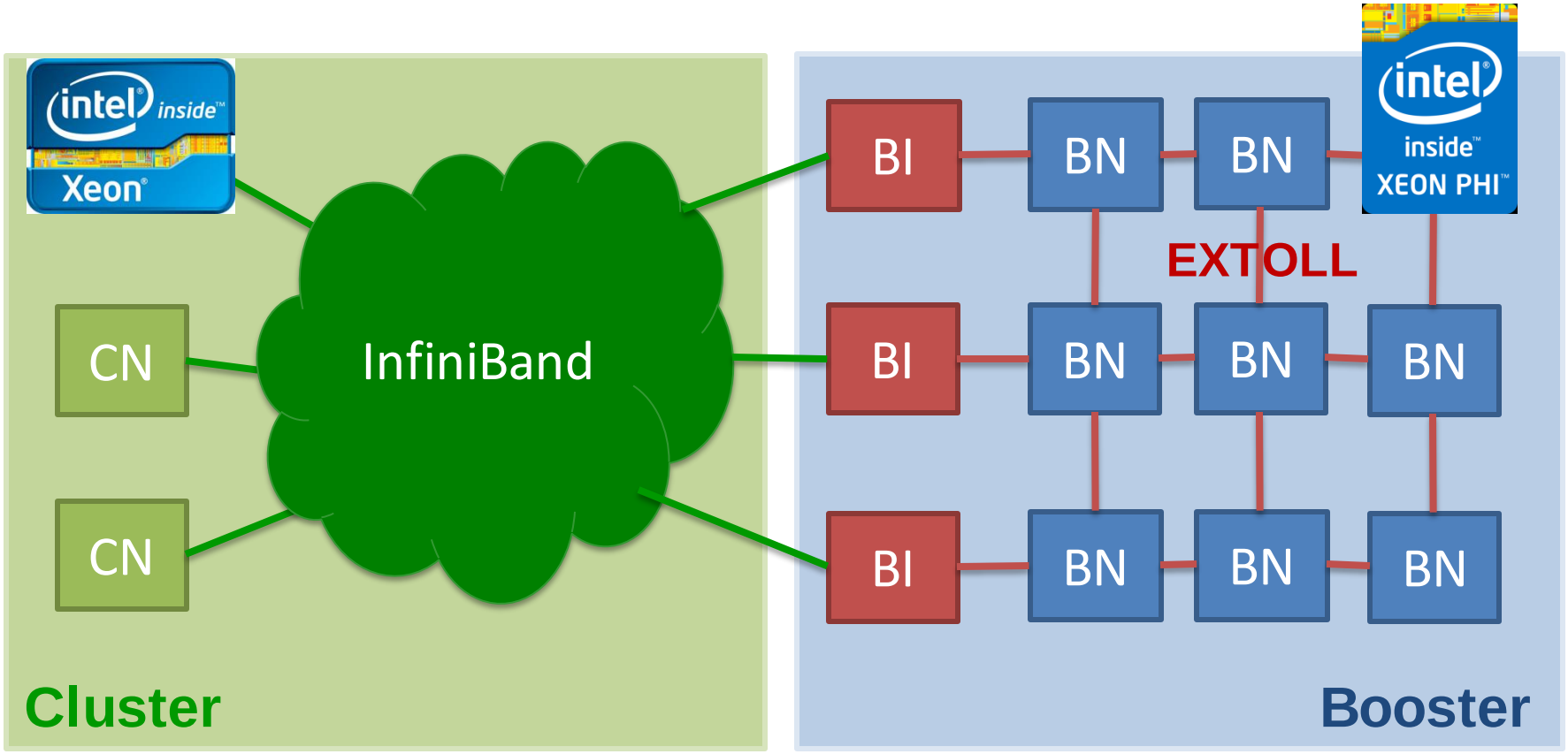
Big Data Analytics

Interactivity

… lead to Modular Supercomputing



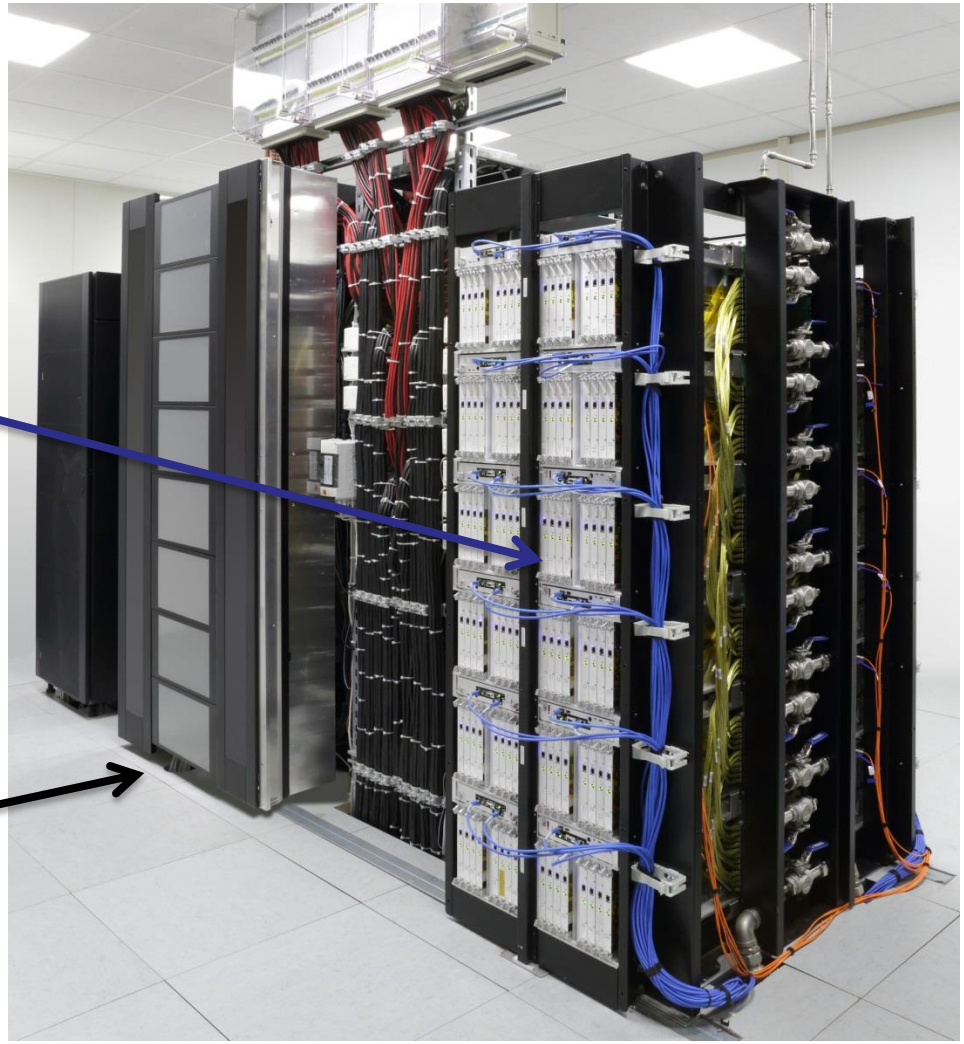
Cluster-Booster Architecture (EU Project DEEP)



Low/Medium scalable code parts

Highly scalable code parts

DEEP Complete System



Neuromorphic and Quantum Computers

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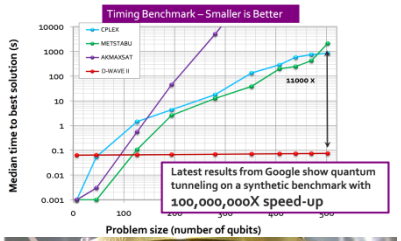
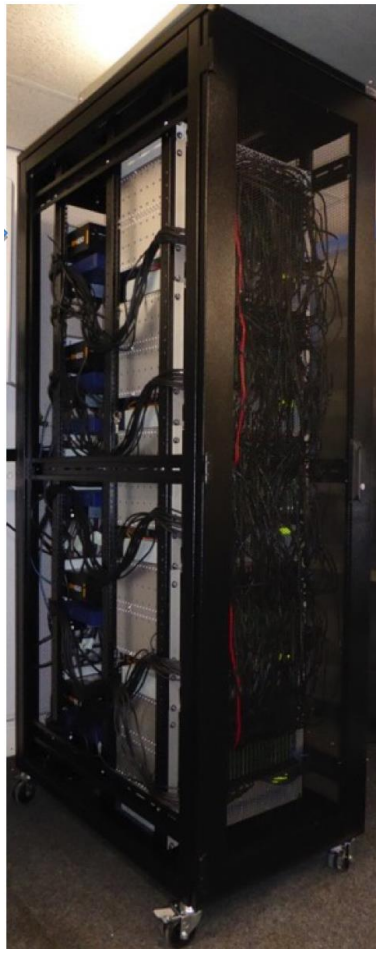
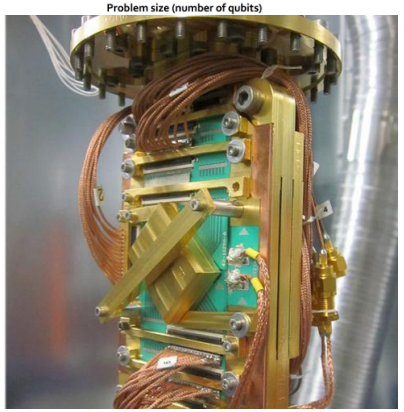
D-Wave Quantum Annealer

$$H_P = -\sum_{i=1}^{N} h_i \sigma_i^z + \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$







BrainScales Neuromorphic Hardware Heidelberg (Karlheinz Meier)

Spinnaker Manchester (Steve Furber)

The new European HPC research landscape